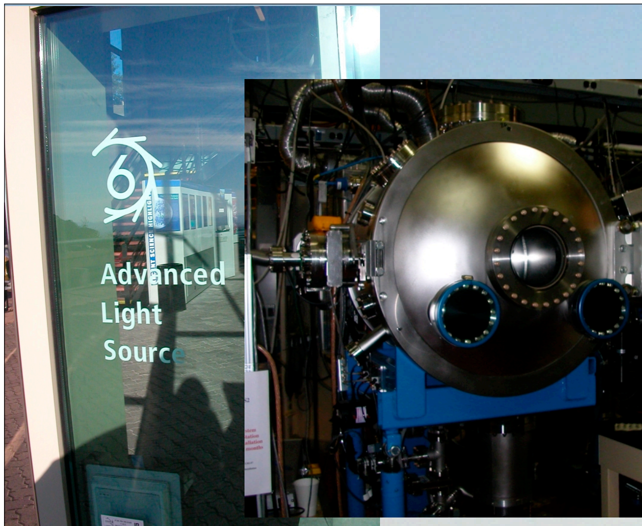
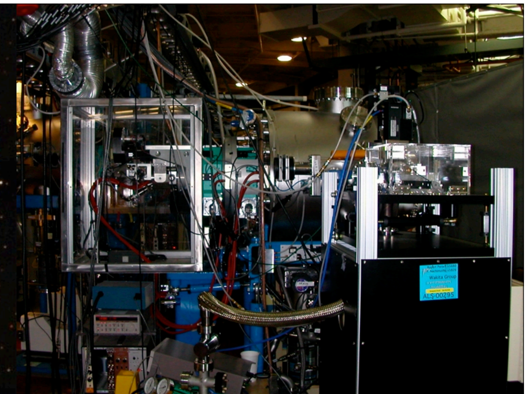




Solid State Astrophysics
Determining the grain composition of the ISM

Julia Lee (Harvard) with Bruce Ravel (ANL)

Constellation-X FST – Cambridge MA 2006 Feb 15-16

Motivation for Dust Studies

- Gets in the way of everything
- Vital to our understanding of the universe
  - dust a primary respository of the ISM
  - interpretation of Cosmology results, etc.
  - chemical evolution of stars, planets, life

Multiwavelength studies of dust

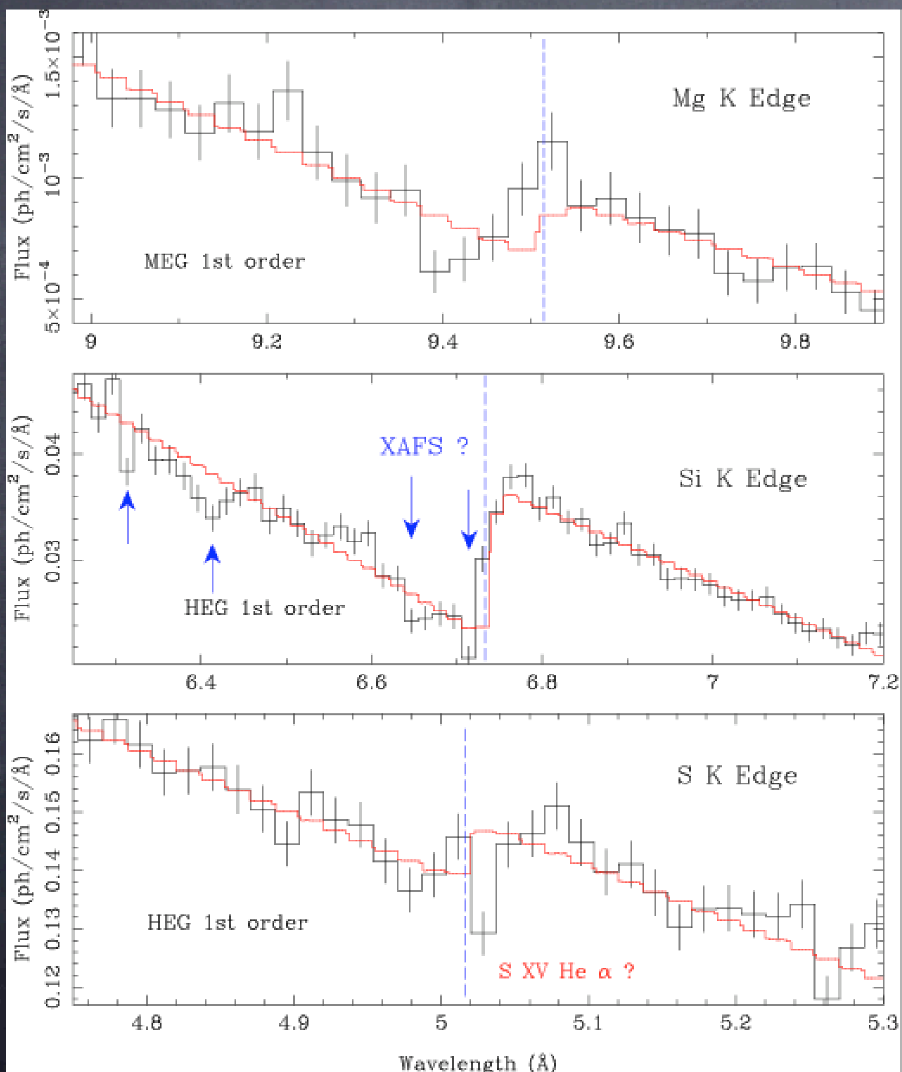
- X-rays : unique probe of solid state nature of molecule; sensitive to ALL atoms in both gas and solid phase
- IR : can directly probe vibrational modes, but limited to PAHs, graphites and certain silicates (~2.5-25 μm region). Cannot easily speciate the grain composition
- UV : dust inferred from the depletion factor (amount expected : measured)
- Optical : dust inferred from redding/extinction, polarization
- Radio : probe gas phase; 21cm, CO, etc.

Reviews, etc from some of the experts

- Dust and Astrophysics :
  - Bruce Draine : Annual Reviews of Astronomy & Astrophysics & references therein: e.g. Li & Greenberg 2003
  - Endrik Krügel : `The Physics of Interstellar Dust'
  - Lyman Spitzer : `Physical Processes in the ISM'
  - D C B Whittet : `Dust in the Galactic Environment'
  - Also, ApJ papers by Woo et al. 1995, 97; Forrey et al. 1998
- XAFS Theory & Practice
  - Koningsberger & Prins (1988)
  - Kruegel (2003)
  - B. Ravel & M. Newville
  - Rehr & Albers (2000)
  - J. Stöhr (1996)

Detections of X-ray Absorption Fine Structure

GRS 1915+105 : Lee et al. 2002



XAFS

EXAFS:
local atomic structure

XANES:
valence of absorber
density of states of abs.

- interstellar grain composition
- solid state astrophysics ?!

also see Ueda et al. 2005

The theory behind measuring X-ray Absorption Fine Structure (XAFS) to determine molecular composition

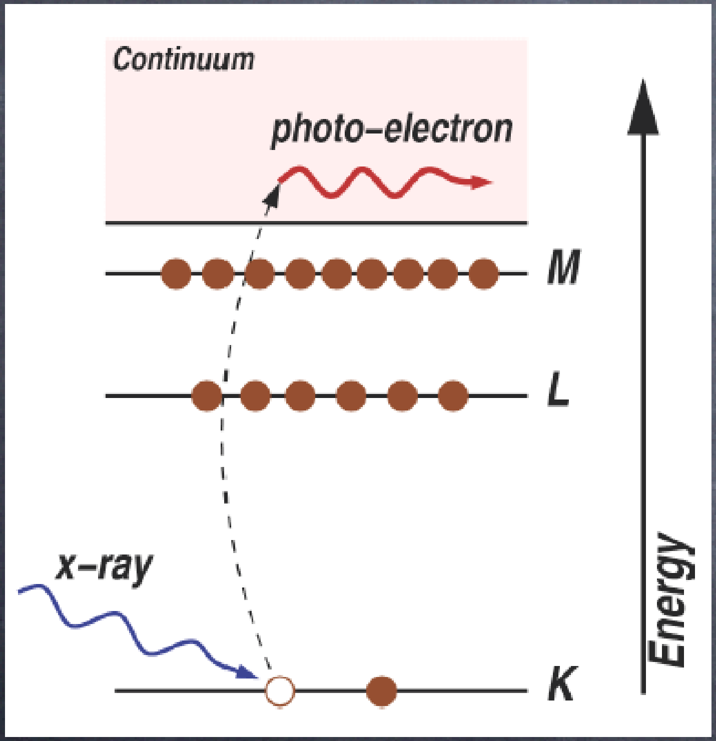
- The photoelectric effect : X-ray photon absorbed by an electron in a tightly bound quantum core level (e.g. 1s or 2p)

Bound-free case for isolated atoms

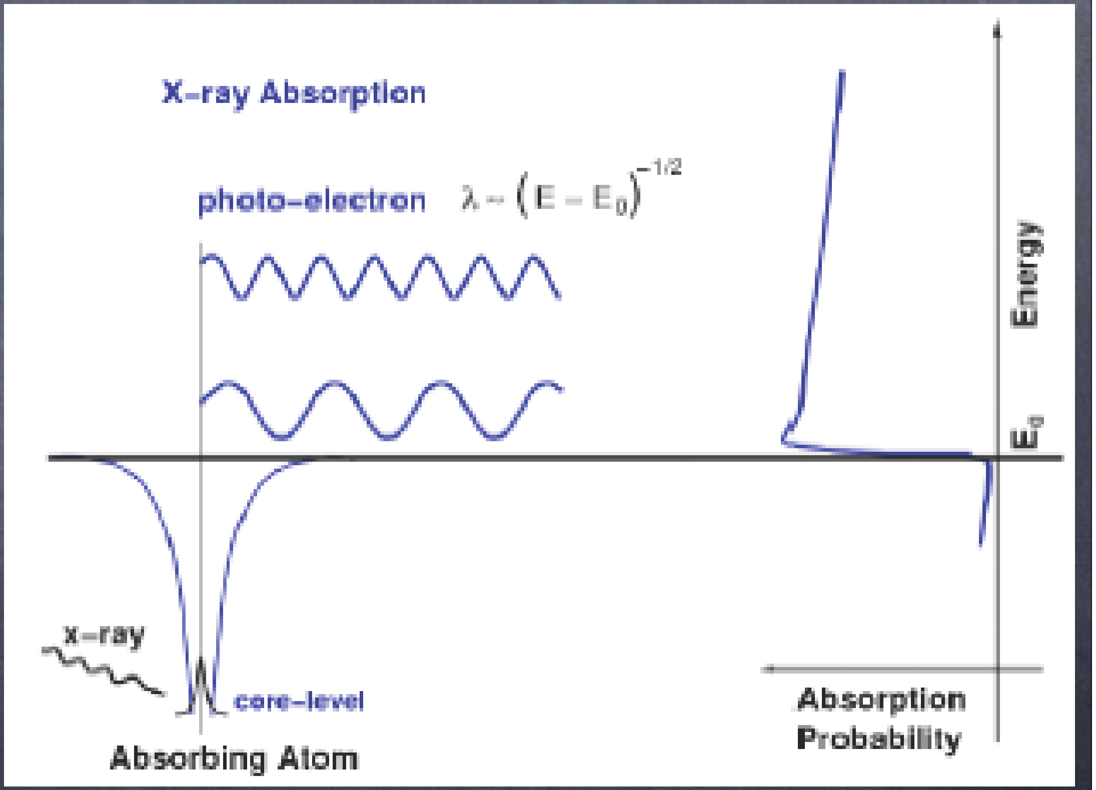
X-ray absorption through the photoelectric process

Isolated Atom: Bound free process --> edge step

promotion of e- to continuum results in sharp rise in the probability for absorption



$$\mu(E) = \mu_0(E)$$

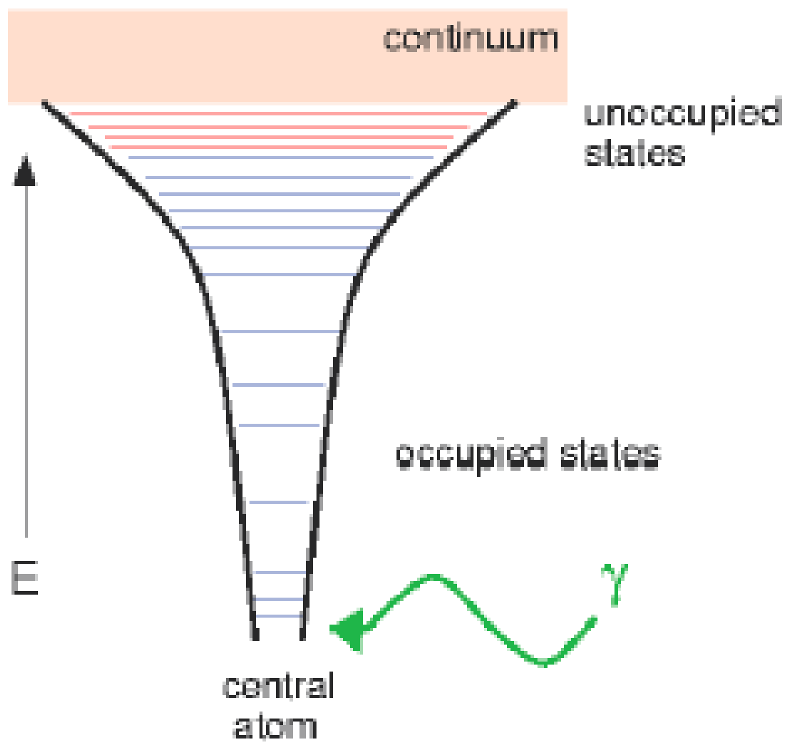


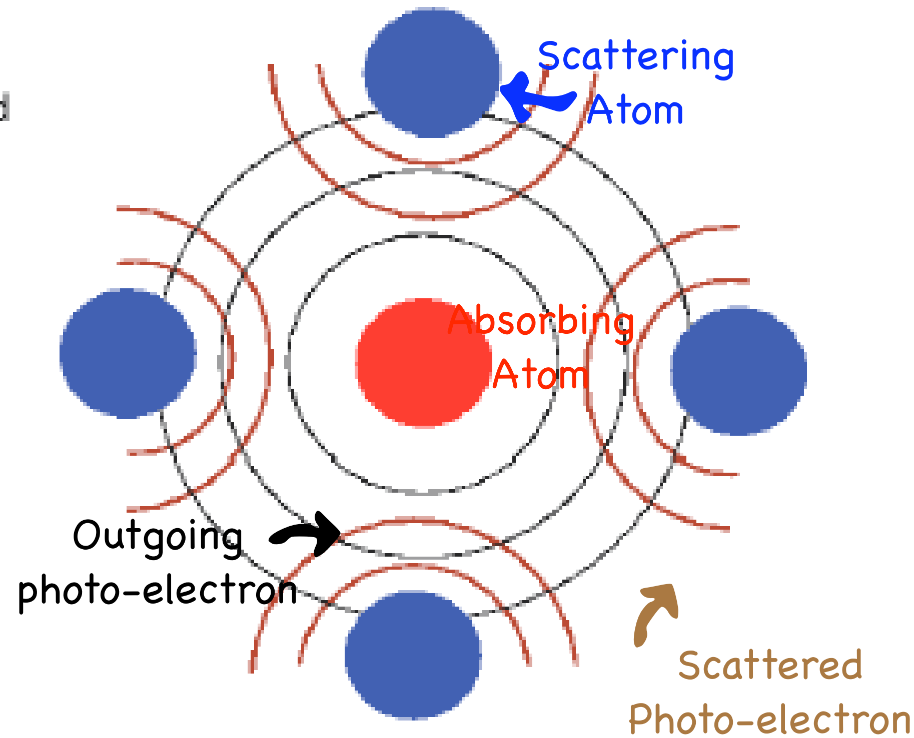
Figures from "XAFS" : © 2002 Matt Newville

The theory behind measuring X-ray Absorption Fine Structure (XAFS) to determine molecular composition

- The photoelectric effect : X-ray photon absorbed by an electron in a tightly bound quantum core level (e.g. 1s or 2p)
- Isolated Atom: Bound free process --> edge step
- Isolated Atom : Bound bound process --> inner shell resonance absorption lines (e.g. MCG-6-30-15: Oxygen V, VI KLL : Lee et al. 2001; IRAS 13349 : 2p-3d M-shell Fe : Sako et al. 2000, NGC 3783 -- Kaspi et al. 2002, Netzer et al. 2003 & references therein; atomic calcs: e.g. Pradhan; Kallman; Behar ...)
- Molecule : bound-bound process --> XAFS

Heuristic Picture of EXAFS



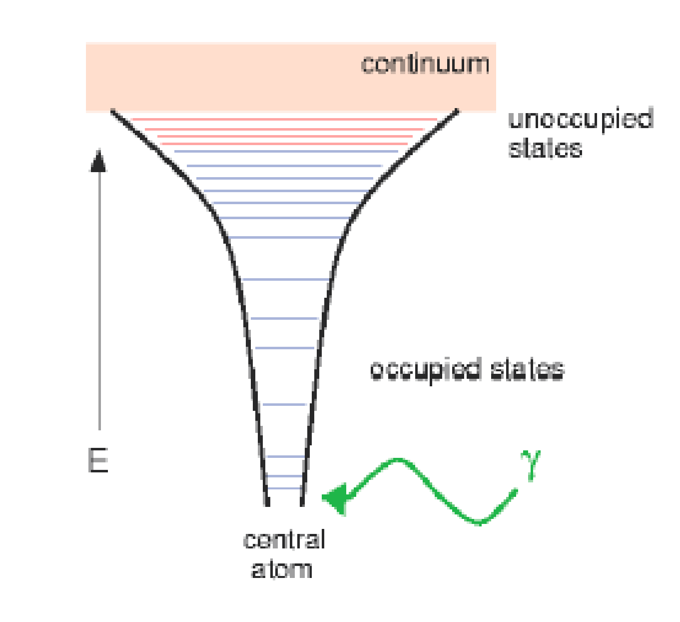


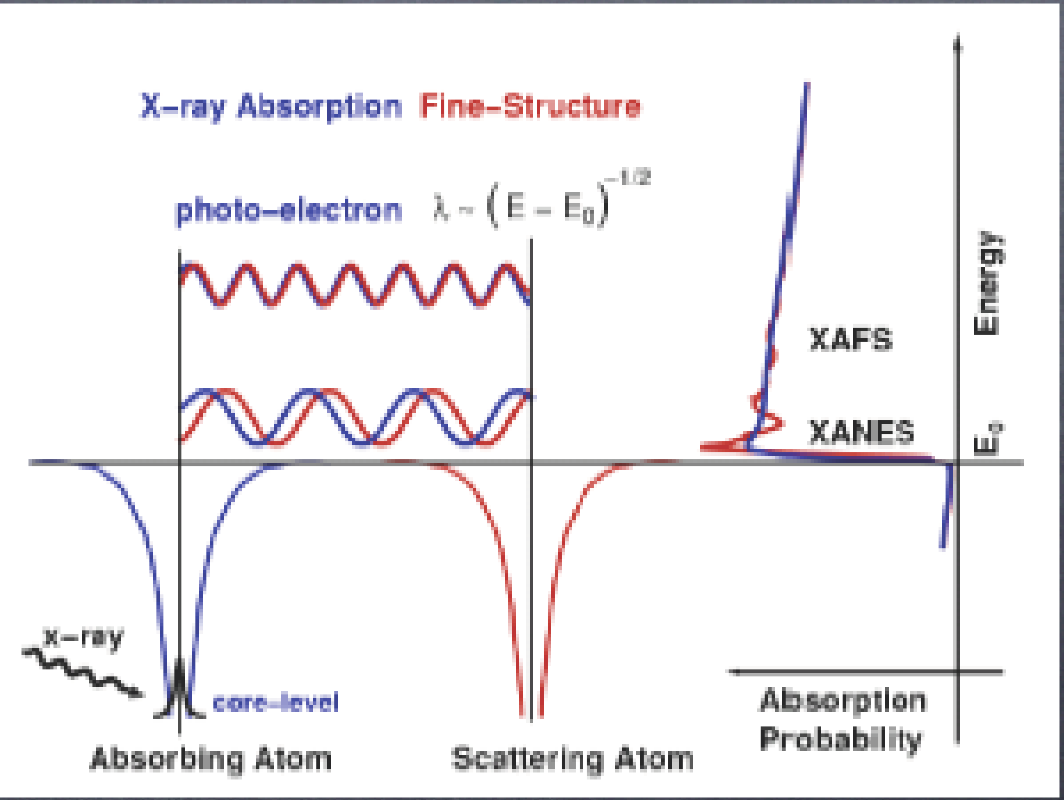
Introduction to EXAFS Analysis Using Theoretical Standard, ©2000-2001 Bruce Ravel

(1) Deep core electron is excited into a state above Fermi energy

(2) Single Scattering Approximation : The photoelectron propagates as a spherical wave & interacts with neighboring atoms -> backscattered wave affects abs. properties of absorbing atom

XAFS Theory
Bound-bound case for molecules





$$\mu(E) = \mu_0(E)[1 + \chi(E)]$$

Figures from "XAFS" : © 2002 Matt Newville

The amplitude of the back-scattered photo-electron at the absorbing atom will vary with energy --> oscillations in μ(E) --> XAFS

The theory behind measuring X-ray Absorption Fine Structure (XAFS) to determine molecular composition

Fermi's Golden Rule :

initial state : an X-ray, a core electron, no photo-election

$$\mu(E) = \mu_0(E)[1+\chi(E)] \propto |< i\,|\,H\,|\,f\ >|^2$$

final state : no X-ray, a core hole, a photo-election

Fine-Structure Term :

depends ONLY on absorbing atom

change in photo-electron final state due to back-scattering from neigboring atom

$$\chi(E) = \frac{\mu(E)-\mu_0(E)}{\Delta\mu_0(E)} \propto < i\,|\,H\,|\,\Delta f >$$

H: interaction term - represents changing between 2 energy, momentum states

photo-electron scattering properties of neighboring atoms

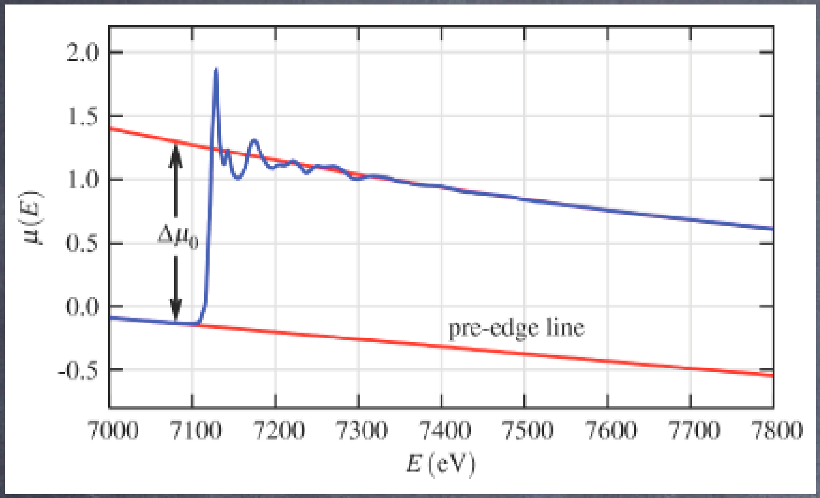
The EXAFS equation :

represents interaction of forward scattering & backscattering photoelectron

$$\chi(\mathrm{k}) = \sum_{\mathrm{j}} \frac{\mathrm{N_j S_0^2 f_j(k) e^{-2R_j/\lambda(k)}\, e^{-2k^2\sigma_j^2}}}{\mathrm{kR_j}^2} \sin[2\mathrm{kR_j} + \delta_{\mathrm{j}}(\mathrm{k})]$$

Single Scattering Approximation

The practice behind measuring X-ray Absorption Fine Structure (XAFS) to determine molecular composition



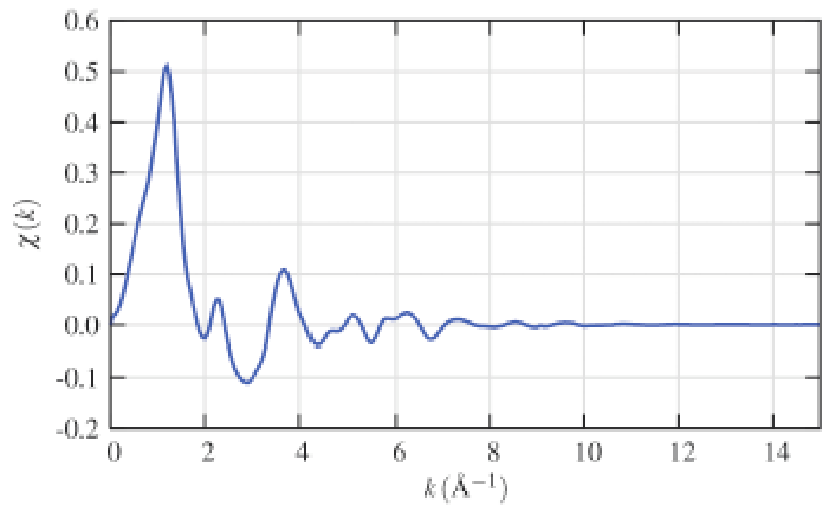
Isolate fine structure term :

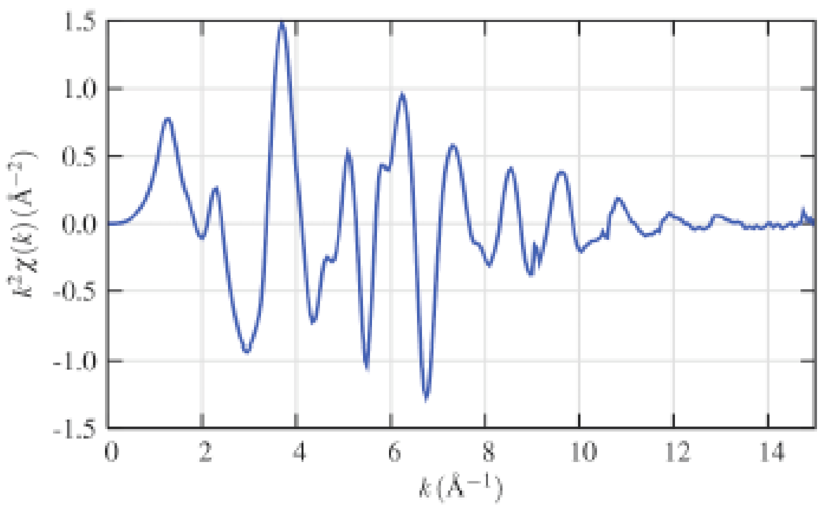
$$\chi(E) = \frac{\mu(E) - \mu_0(E)}{\Delta\mu_0(E)} \propto < i \,|\, H \,|\, \Delta f >$$

interference effect : depends on wave nature of photoelectron

$$\chi(E) \longrightarrow \chi(k)$$

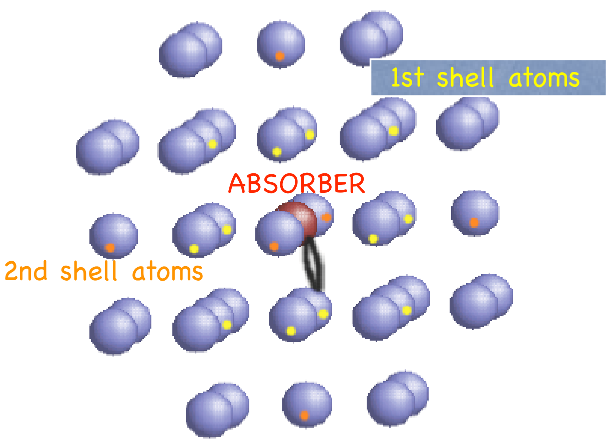
$$\mathbf{k} = \sqrt{\frac{\mathbf{2m(E - E_0)}}{\hbar^2}}$$

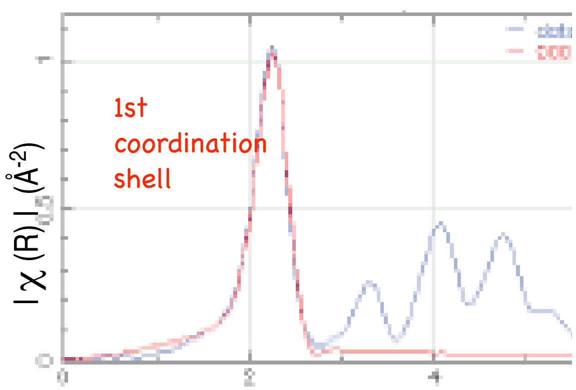




Scattering Paths

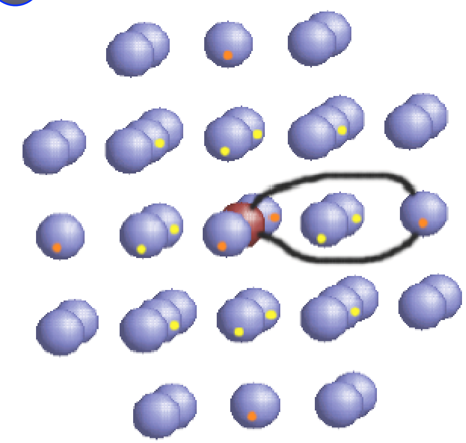
1 Single Scattering Path

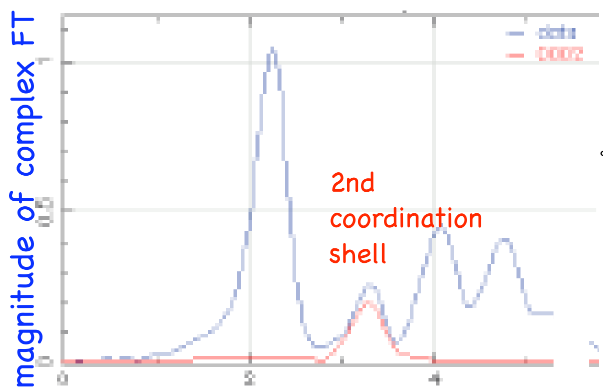




Radial Distance from Absorbing Atom (Å)

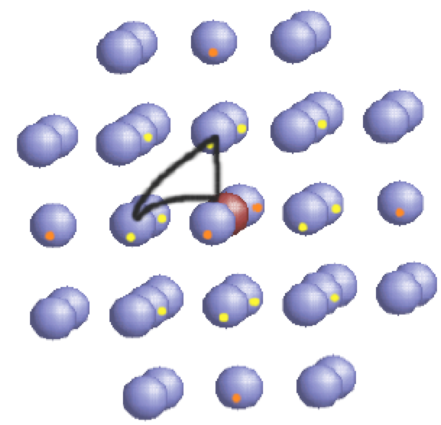
2 Single Scattering Path

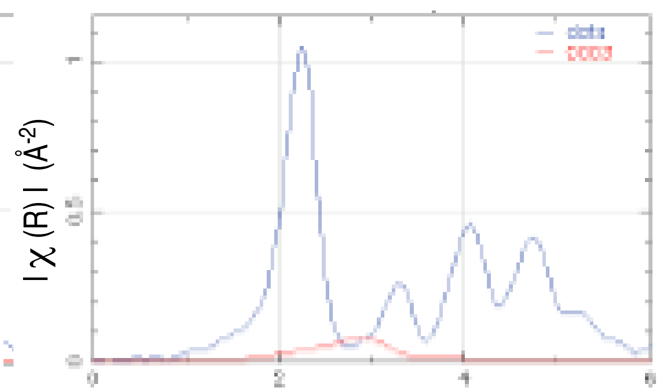




Radial Distance from Absorbing Atom (Å)

3 Double Scattering Path ...



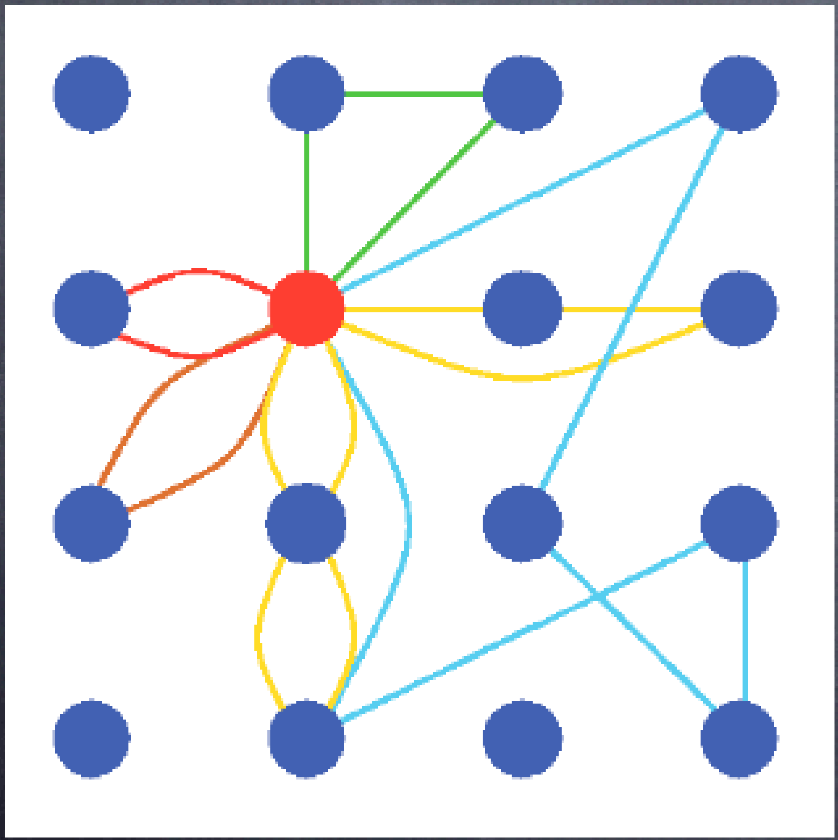


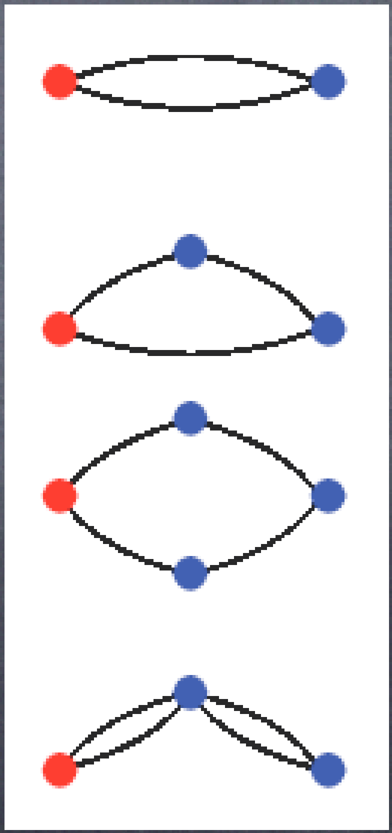
Radial Distance from Absorbing Atom (Å)

$$\chi(k) = \sum_j \frac{N_j S_0^2 f_j(k) e^{-2R_j/\lambda(k)}\, e^{-2k^2\sigma_j^2}}{kR_j{}^2} \sin[2kR_j + \delta_j(k)]$$

Scattering Paths

$$\chi(k) = \sum_i \frac{S_0^2 F_i(k)}{2kR_i^2} \, e^{-2\sigma_i^2 k^2} \, e^{-2R_i/\lambda(k)} \sin[2kR_i + \Phi_i(k)]$$

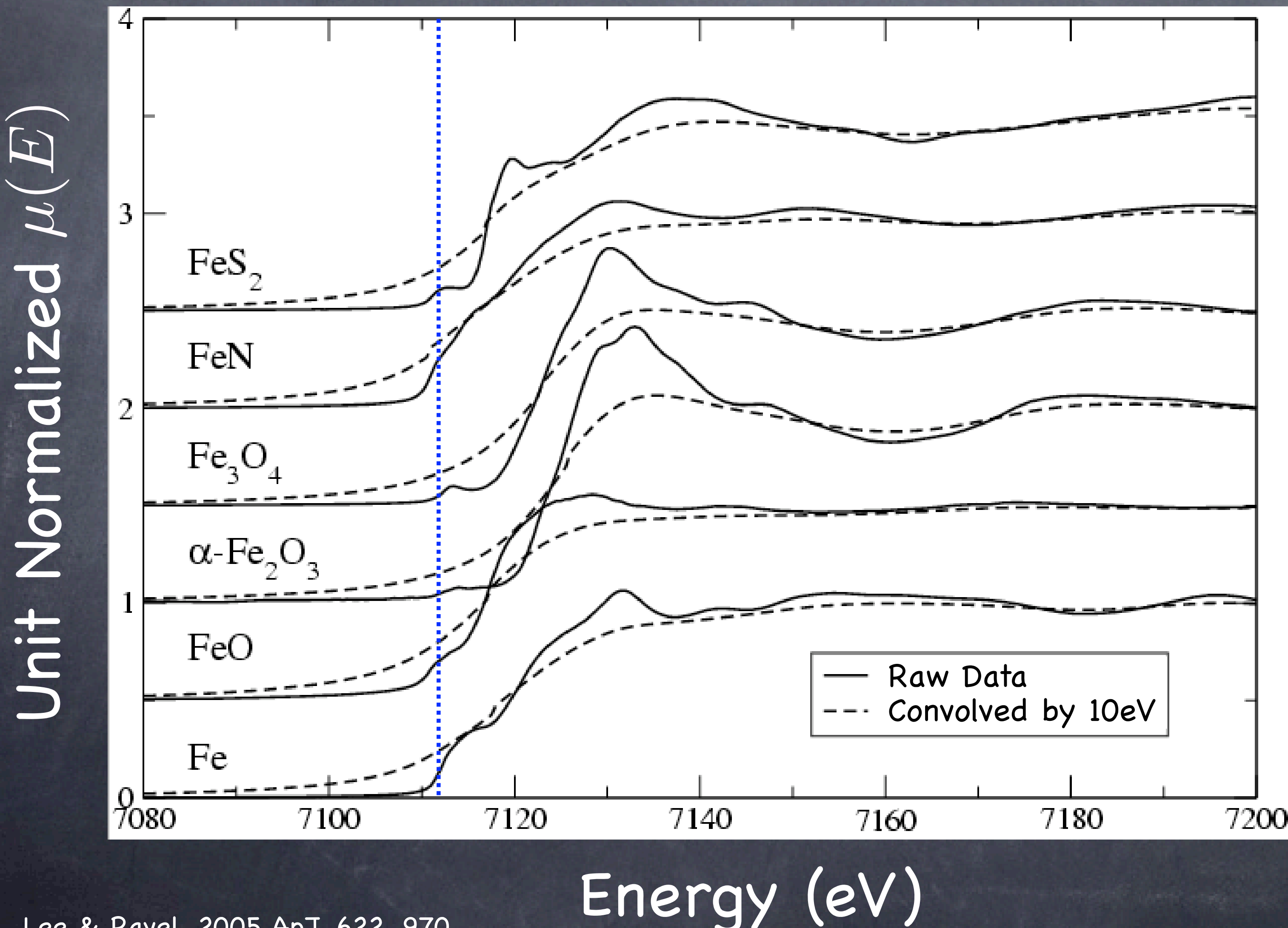




ISM Grain Candidates

- UV, IR, & meteorite studies indicate compositions :
  - ice : H_2O
  - graphite : C
  - polyaromatic hydrocarbons : PAHs
  - silicates : SiO_2, $FeSiO_3$, $FeSiO_4$, $MgSiO_3$, Mg_2SiO_4
  - iron species : Fe, FeO, Fe_2O_3, Fe_3O_4

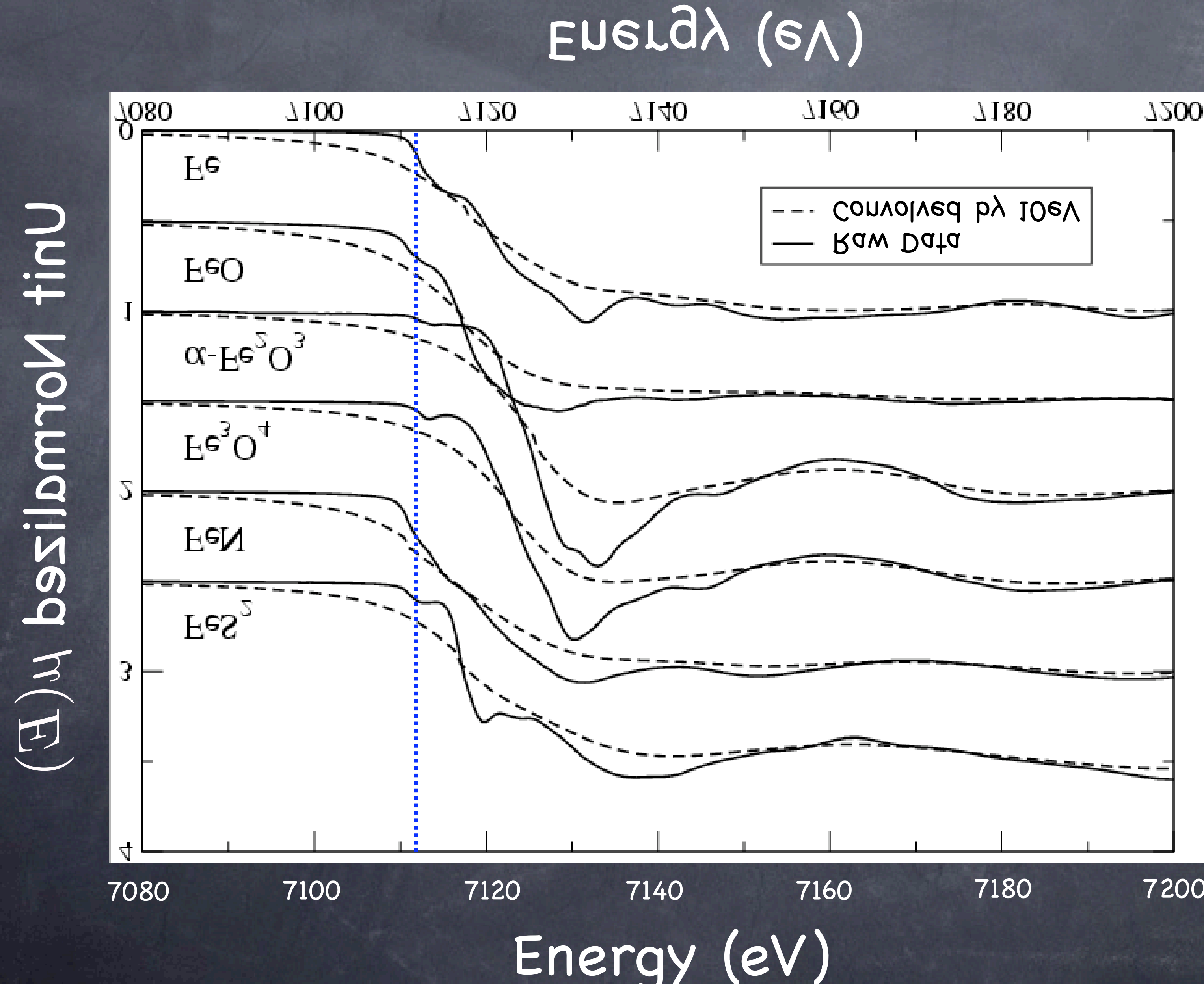
K-edge Absorption Cross Sections for IRON compounds



Data from BNL National Synchrotron Light Source and Argonne National Laboratory Advanced Photon Source

Lee & Ravel, 2005 ApJ. 622, 970

For us Astronomers ...



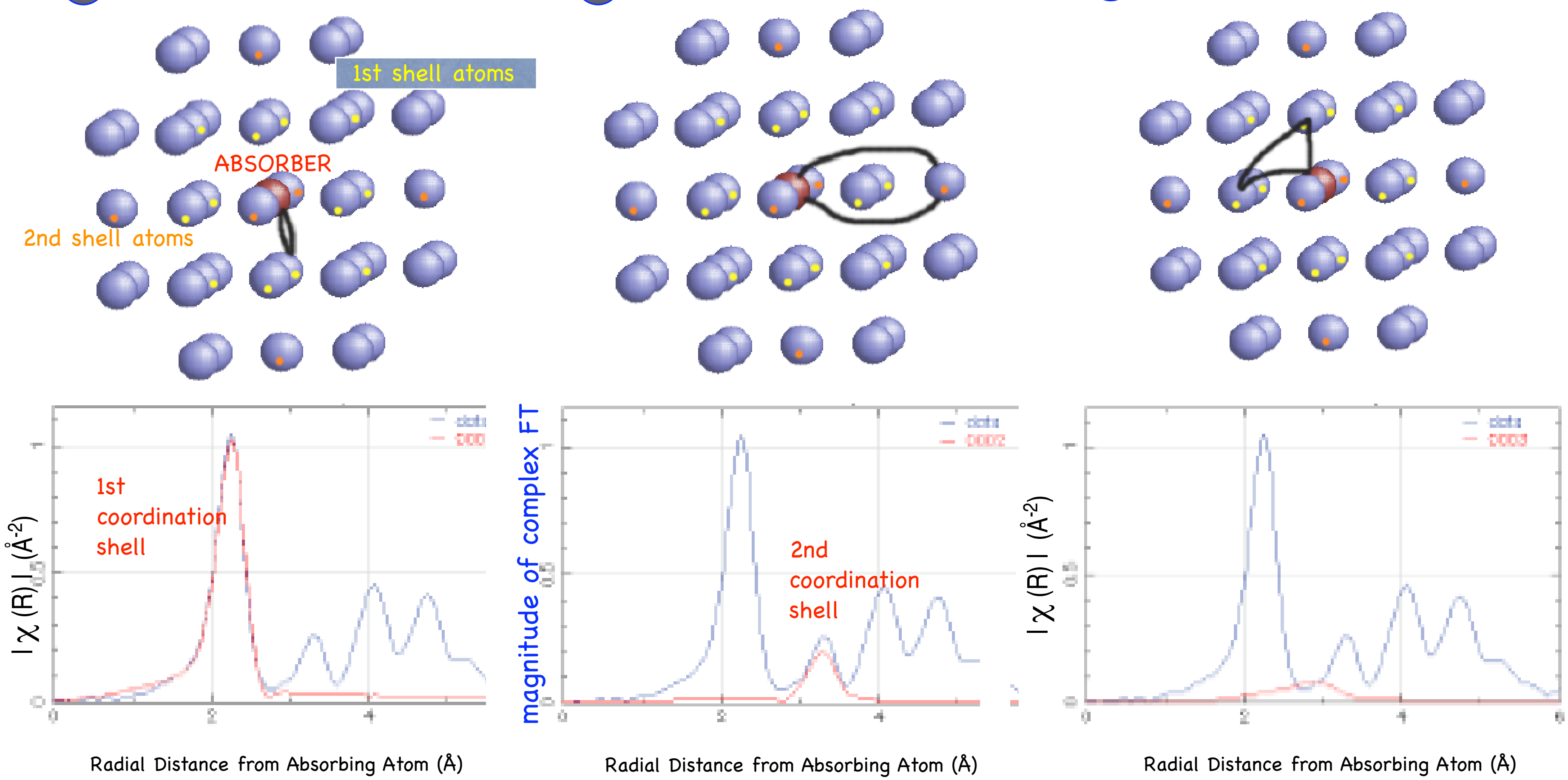
Data from BNL National Synchrotron Light Source beamline X11A

Scattering Paths

1 Single Scattering Path

2 Single Scattering Path

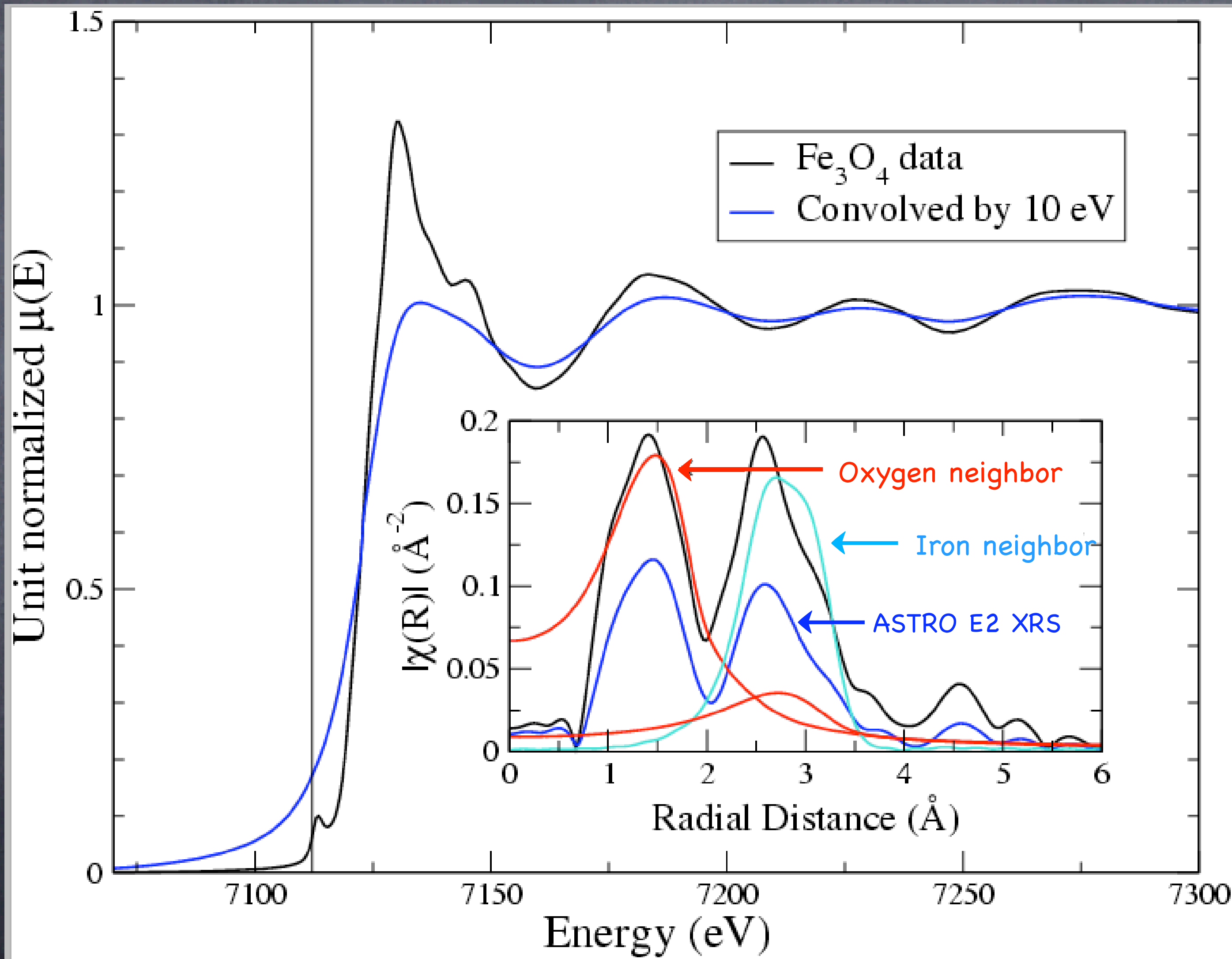
3 Double Scattering Path ...



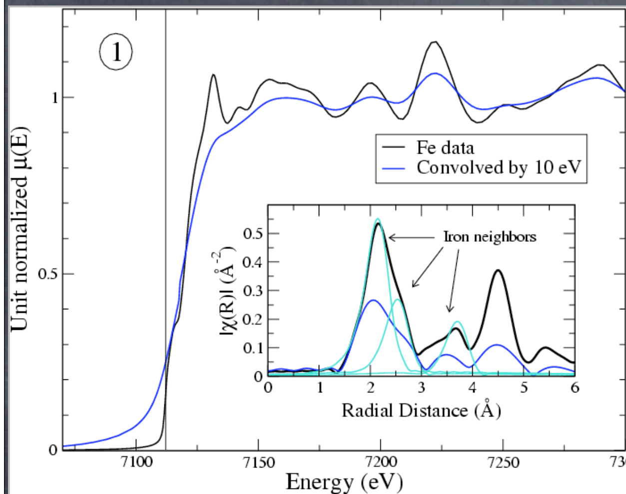
$$\chi(k) = \sum_j \frac{N_j S_0^2 f_j(k) e^{-2R_j/\lambda(k)}\, e^{-2k^2\sigma_j^2}}{kR_j{}^2} \sin[2kR_j + \delta_j(k)]$$

Identifying Compounds using XAFS theory and synchrotron analysis techniques

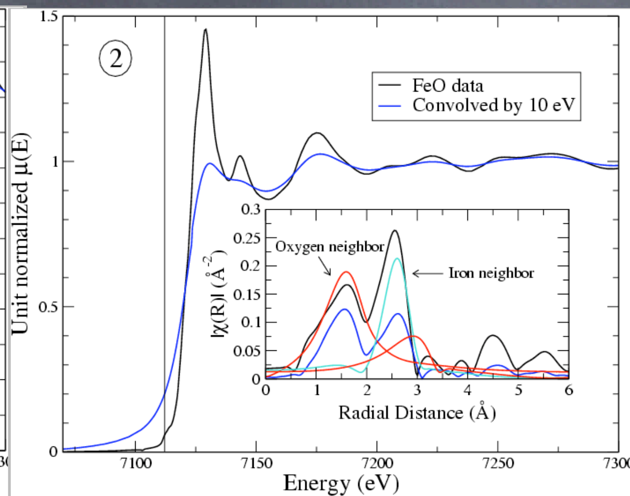
Data from BNL National Synchrotron Light Source and Argonne National Laboratory Advanced Photon Source



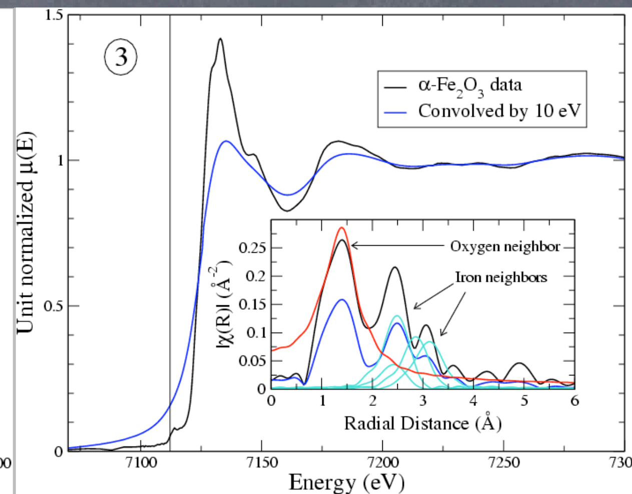
metallic iron



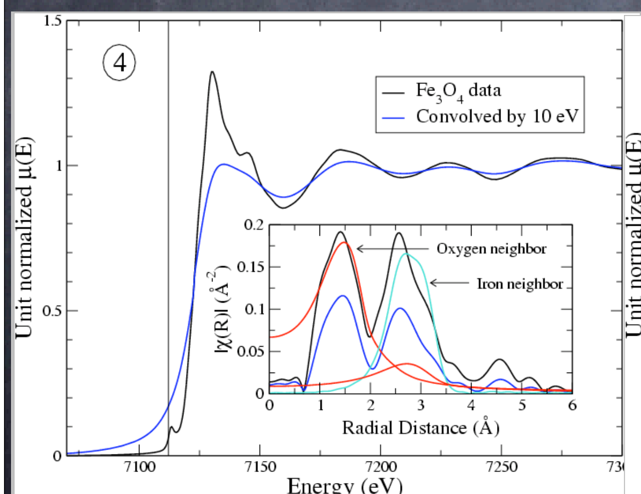
wüstite



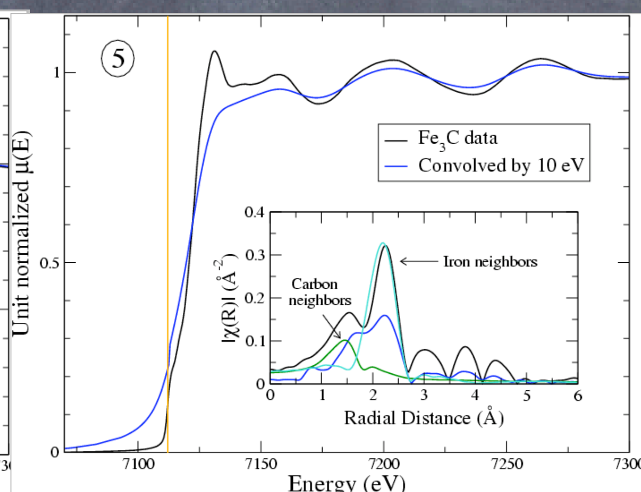
hematite



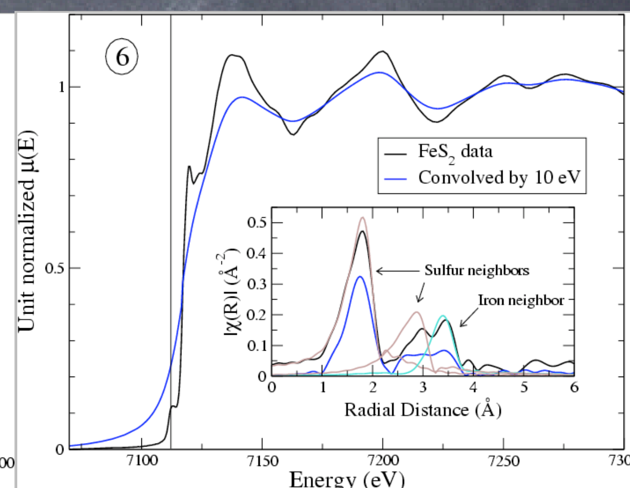
magnetite



iron carbide



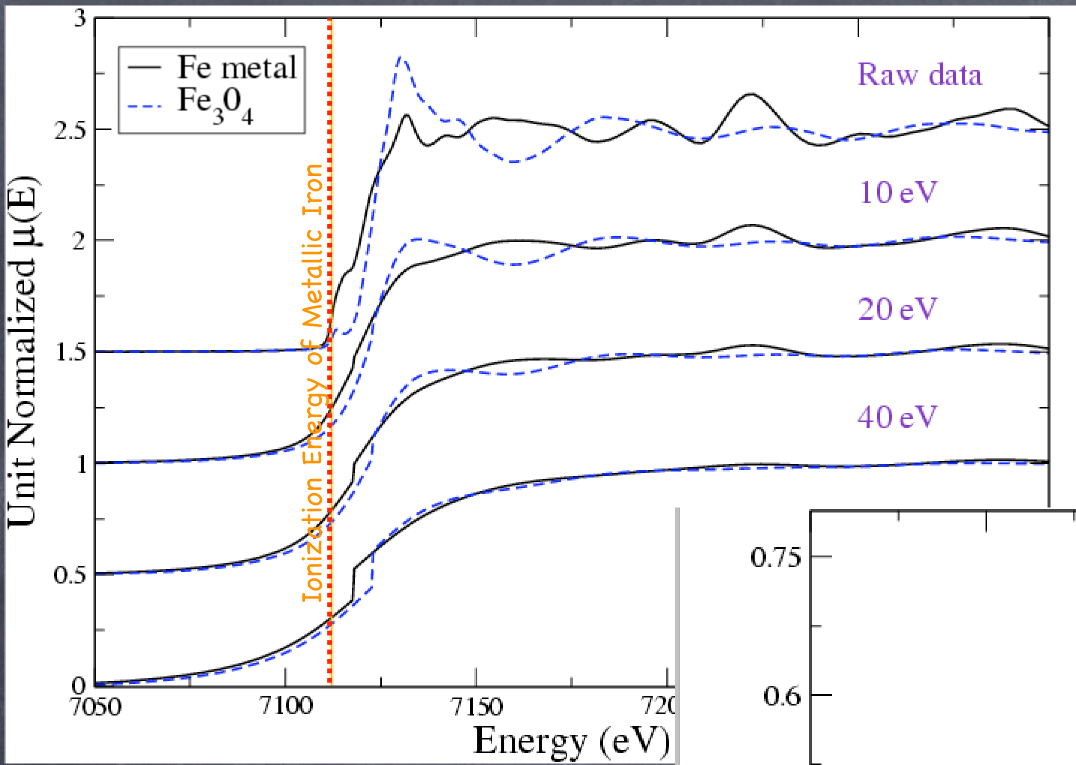
pyrite

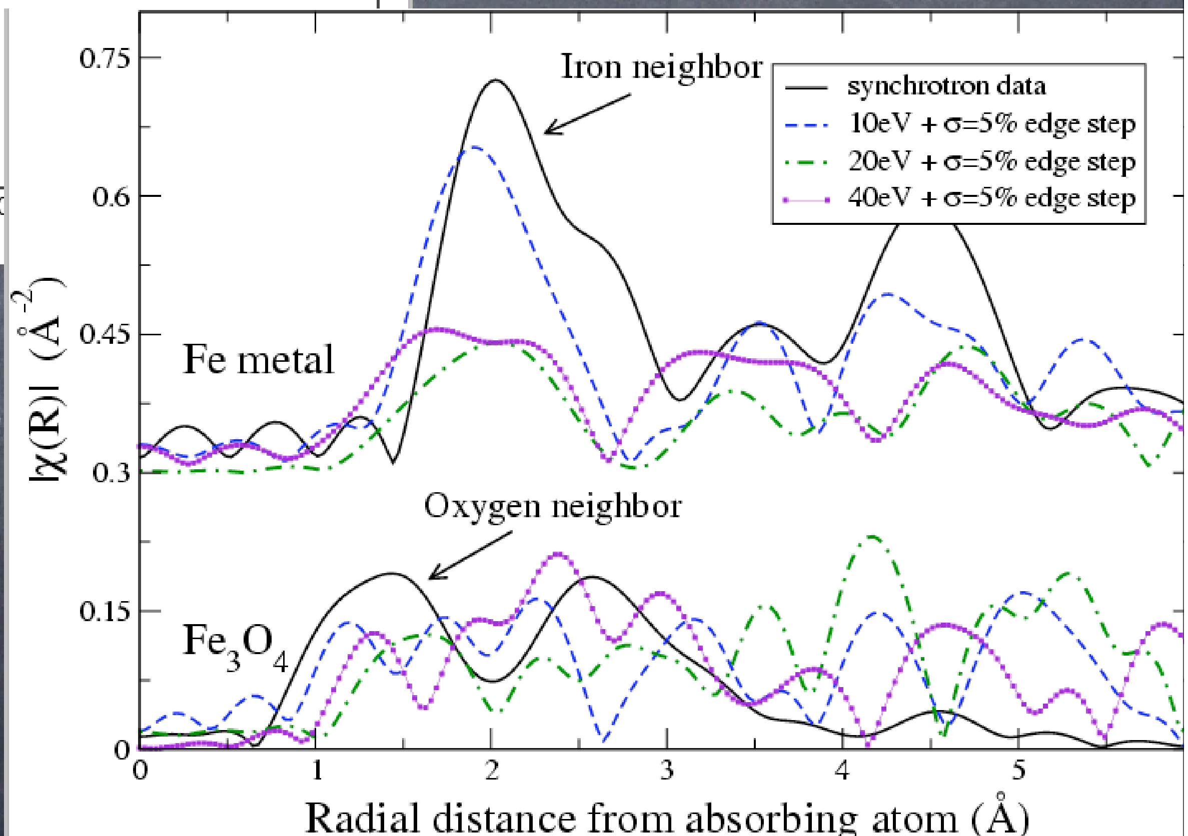


Lee & Ravel, 2005 ApJ. 622, 970

Lee & Ravel 2005 ApJ

The limiting effects of spectral resolution





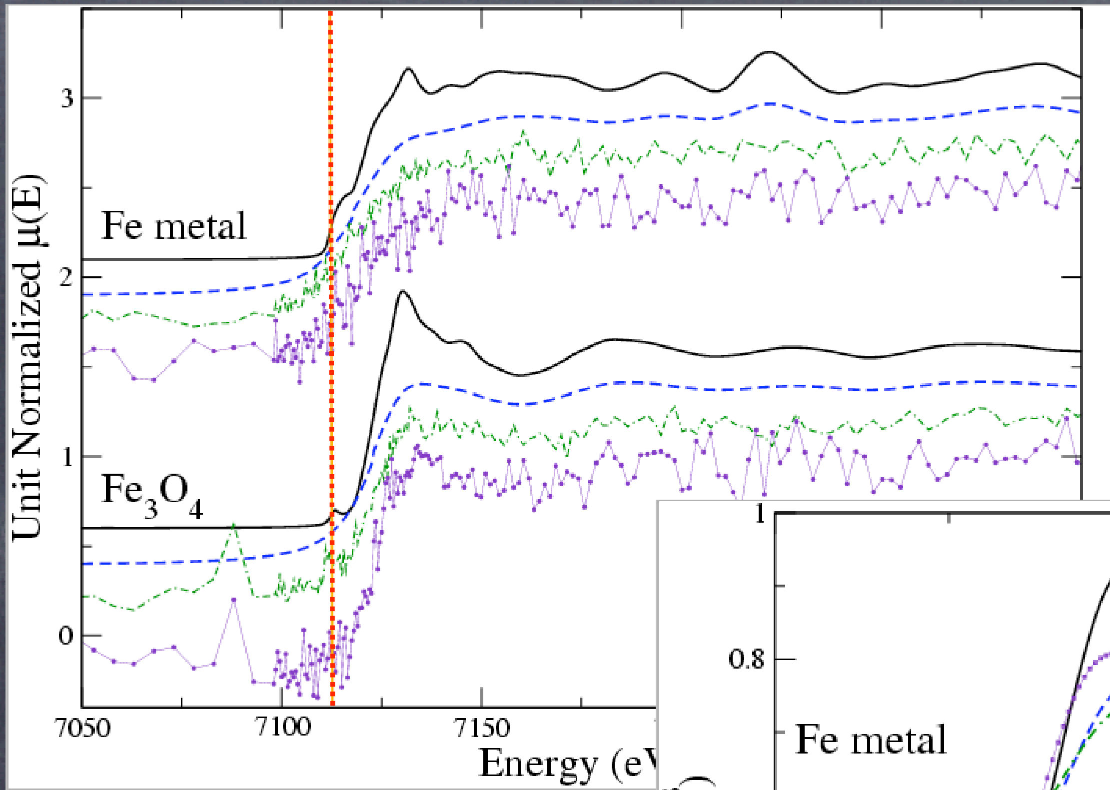
At moderate noise level

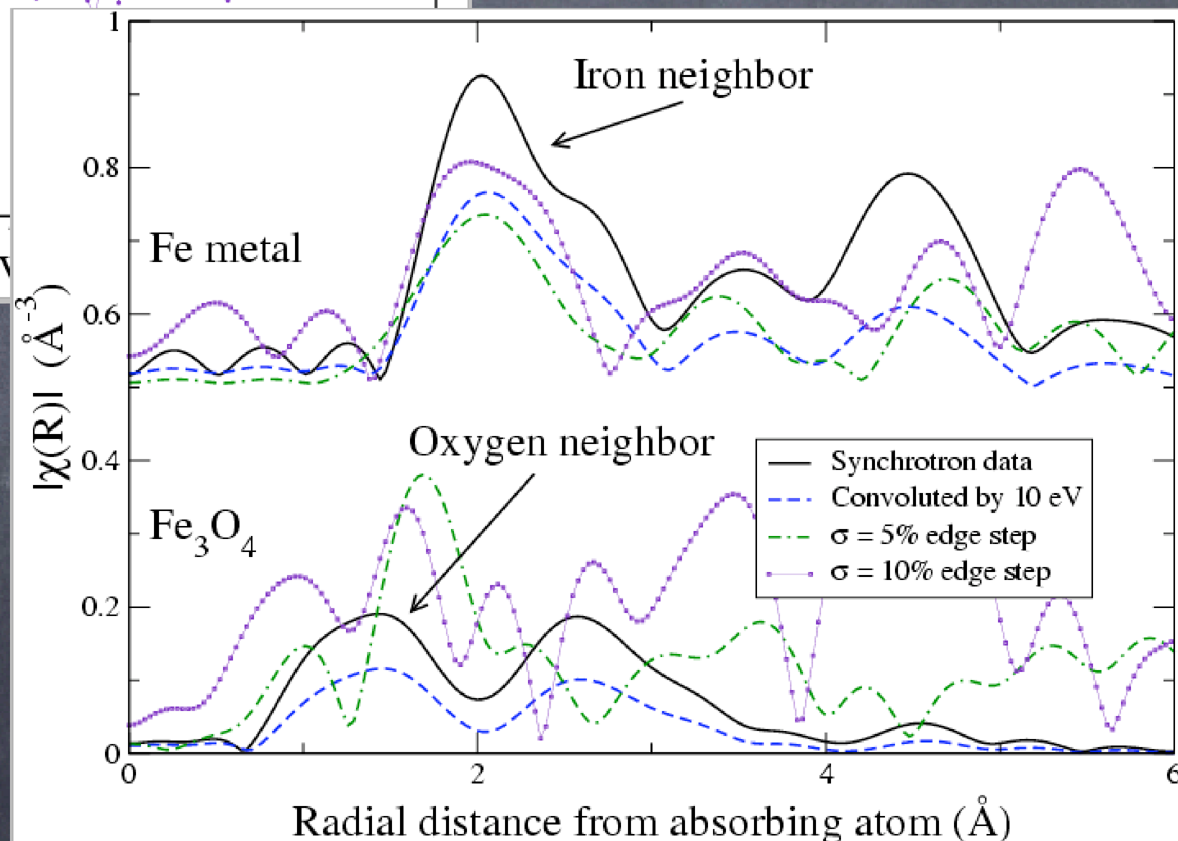
Fe Metal :
R = 20 eV maybe still OK

Magnetite :
R = 10 eV a minimum

Data from BNL NSLS & ANL APS

The limiting effects of noise





Lee & Ravel 2005 ApJ

At R~10 eV

Fe Metal :
can tolerate relatively high noise

Magnetite :
cannot even tolerate 5% noise

Data from BNL NSLS X11A beamline

Constellation-X and ISM Grain Physics
Need AREA + Spectral R >= 2500-3000

	Gratings 0.25 - 6 keV FWHM			Calorimeter 6-10 keV FWHM		
	$E/\Delta E=300$ Baseline Con-X	$E/\Delta E=1000$ Chandra	Ideal $E/\Delta E$	$E/\Delta E \sim 923$ Suzaku	$E/\Delta E= 1500$ Baseline Con-X	Ideal $E/\Delta E$
Gas vs. dust	Difficult without context	YES (isolate WA though)		YES	YES	
Different dust	NO WAY !	MAYBE, with good statistics	3000 silicates from Fe/oxides but $Fe_3O_4 = Fe_2O_3$	OK with good statistics	silicates from iron / oxides	3000
Discern oxides	NO WAY !	NO	5000	NO	very hard to not possible	5000